

Supporting Information for 2-
Indolylphosphines: A New Class of Tunable
Ligands – Their Syntheses, Facile
Derivatization, and Coordination to Pd(II)

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Additional Material: [P(C₆H₅)₂(C₉H₈N)] (1)

Table 1. Crystal data and structure refinement for k0191.

Identification code	k0191	
Empirical formula	C ₂₁ H ₁₈ N P	
Formula weight	315.33	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.9678(2) Å	α = 79.973(8)°.
	b = 10.3453(2) Å	β = 75.992(7)°.
	c = 17.4704(4) Å	γ = 74.133(9)°.
Volume	1670.09(6) Å ³	
Z	4	
Density (calculated)	1.254 Mg/m ³	
Absorption coefficient	0.163 mm ⁻¹	
F(000)	664	
Crystal size	0.35 x 0.30 x 0.30 mm ³	
Theta range for data collection	2.55 to 27.48°.	
Index ranges	0 ≤ h ≤ 12, -12 ≤ k ≤ 13, -21 ≤ l ≤ 22	
Reflections collected	22759	
Independent reflections	7596 [R(int) = 0.046]	
Completeness to theta = 27.51°	99.1 %	
Max. and min. transmission	0.9526 and 0.9450	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7596 / 0 / 426	
Goodness-of-fit on F ²	1.057	
Final R indices [I > 2σ(I)]	R1 = 0.0449, wR2 = 0.1140	
R indices (all data)	R1 = 0.0767, wR2 = 0.1320	
Extinction coefficient	0.0014(16)	
Largest diff. peak and hole	0.257 and -0.258 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k0191. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
P(1A)	7112(1)	6342(1)	850(1)	29(1)
P(1B)	3540(1)	2753(1)	4637(1)	36(1)
N(1A)	4120(2)	6627(2)	1081(1)	31(1)
N(1B)	740(2)	2401(2)	4843(1)	36(1)
C(2A)	5244(2)	7224(2)	1031(1)	30(1)
C(2B)	2160(2)	2102(2)	4440(1)	33(1)
C(3A)	4709(2)	8591(2)	1061(1)	30(1)
C(3B)	2295(2)	1346(2)	3841(1)	33(1)
C(4A)	3196(2)	8856(2)	1123(1)	31(1)
C(4B)	901(2)	1177(2)	3866(1)	33(1)
C(5A)	2115(2)	10048(2)	1144(1)	44(1)
C(5B)	362(2)	551(2)	3395(1)	43(1)
C(6A)	744(2)	9960(2)	1183(2)	54(1)
C(6B)	-1062(3)	560(2)	3591(2)	51(1)
C(7A)	427(2)	8711(2)	1212(1)	48(1)
C(7B)	-1972(2)	1170(2)	4248(1)	46(1)
C(8A)	1471(2)	7514(2)	1203(1)	38(1)
C(8B)	-1476(2)	1801(2)	4713(1)	41(1)
C(9A)	2859(2)	7611(2)	1144(1)	31(1)
C(9B)	-37(2)	1816(2)	4510(1)	34(1)
C(10A)	5530(2)	9621(2)	1023(1)	40(1)
C(10B)	3630(2)	771(2)	3274(1)	45(1)
C(11A)	7525(2)	6355(2)	-234(1)	27(1)
C(11B)	2750(2)	3175(2)	5653(1)	33(1)
C(12A)	8927(2)	6323(2)	-630(1)	31(1)
C(12B)	2848(2)	2116(2)	6270(1)	43(1)
C(13A)	9311(2)	6377(2)	-1450(1)	36(1)
C(13B)	2286(3)	2363(2)	7051(1)	49(1)
C(14A)	8296(2)	6471(2)	-1893(1)	36(1)
C(14B)	1641(2)	3666(2)	7238(1)	44(1)
C(15A)	6894(2)	6512(2)	-1508(1)	35(1)

C(15B)	1552(2)	4726(2)	6635(1)	40(1)
C(16A)	6511(2)	6459(2)	-689(1)	31(1)
C(16B)	2095(2)	4484(2)	5849(1)	37(1)
C(17A)	6958(2)	4601(2)	1211(1)	27(1)
C(17B)	3269(2)	4431(2)	4064(1)	34(1)
C(18A)	6565(2)	4273(2)	2032(1)	33(1)
C(18B)	2096(2)	5041(2)	3713(1)	40(1)
C(19A)	6521(2)	2959(2)	2353(1)	37(1)
C(19B)	1996(3)	6296(2)	3264(1)	48(1)
C(20A)	6867(2)	1950(2)	1858(1)	37(1)
C(20B)	3065(3)	6968(2)	3169(1)	48(1)
C(21A)	7250(2)	2261(2)	1045(1)	35(1)
C(21B)	4217(2)	6393(2)	3526(1)	45(1)
C(22A)	7296(2)	3578(2)	721(1)	29(1)
C(22B)	4330(2)	5130(2)	3962(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for k0191.

P(1A)-C(2A)	1.8127(19)
P(1A)-C(17A)	1.8367(18)
P(1A)-C(11A)	1.8376(19)
P(1B)-C(2B)	1.811(2)
P(1B)-C(17B)	1.833(2)
P(1B)-C(11B)	1.835(2)
N(1A)-C(9A)	1.378(2)
N(1A)-C(2A)	1.399(2)
N(1B)-C(9B)	1.378(2)
N(1B)-C(2B)	1.396(2)
C(2A)-C(3A)	1.374(3)
C(2B)-C(3B)	1.372(3)
C(3A)-C(4A)	1.438(3)
C(3A)-C(10A)	1.495(3)
C(3B)-C(4B)	1.437(3)
C(3B)-C(10B)	1.497(3)
C(4A)-C(5A)	1.397(3)
C(4A)-C(9A)	1.409(3)
C(4B)-C(5B)	1.404(3)
C(4B)-C(9B)	1.410(3)
C(5A)-C(6A)	1.380(3)
C(5B)-C(6B)	1.375(3)
C(6A)-C(7A)	1.402(3)
C(6B)-C(7B)	1.404(3)
C(7A)-C(8A)	1.382(3)
C(7B)-C(8B)	1.373(3)
C(8A)-C(9A)	1.392(3)
C(8B)-C(9B)	1.396(3)
C(11A)-C(12A)	1.396(2)
C(11A)-C(16A)	1.400(3)
C(11B)-C(16B)	1.396(3)
C(11B)-C(12B)	1.398(3)
C(12A)-C(13A)	1.385(3)
C(12B)-C(13B)	1.383(3)

C(13A)-C(14A)	1.389(3)
C(13B)-C(14B)	1.385(3)
C(14A)-C(15A)	1.390(3)
C(14B)-C(15B)	1.382(3)
C(15A)-C(16A)	1.385(3)
C(15B)-C(16B)	1.388(3)
C(17A)-C(22A)	1.395(2)
C(17A)-C(18A)	1.398(3)
C(17B)-C(18B)	1.397(3)
C(17B)-C(22B)	1.399(3)
C(18A)-C(19A)	1.385(3)
C(18B)-C(19B)	1.387(3)
C(19A)-C(20A)	1.390(3)
C(19B)-C(20B)	1.388(3)
C(20A)-C(21A)	1.382(3)
C(20B)-C(21B)	1.380(3)
C(21A)-C(22A)	1.391(3)
C(21B)-C(22B)	1.383(3)
C(2A)-P(1A)-C(17A)	99.94(8)
C(2A)-P(1A)-C(11A)	101.64(8)
C(17A)-P(1A)-C(11A)	102.97(8)
C(2B)-P(1B)-C(17B)	101.94(9)
C(2B)-P(1B)-C(11B)	100.44(9)
C(17B)-P(1B)-C(11B)	101.59(9)
C(9A)-N(1A)-C(2A)	109.28(16)
C(9B)-N(1B)-C(2B)	109.10(16)
C(3A)-C(2A)-N(1A)	108.95(16)
C(3A)-C(2A)-P(1A)	126.14(14)
N(1A)-C(2A)-P(1A)	124.60(13)
C(3B)-C(2B)-N(1B)	109.06(17)
C(3B)-C(2B)-P(1B)	126.48(15)
N(1B)-C(2B)-P(1B)	124.25(14)
C(2A)-C(3A)-C(4A)	106.78(16)
C(2A)-C(3A)-C(10A)	127.17(18)
C(4A)-C(3A)-C(10A)	126.04(17)

C(2B)-C(3B)-C(4B)	106.96(17)
C(2B)-C(3B)-C(10B)	127.42(19)
C(4B)-C(3B)-C(10B)	125.61(18)
C(5A)-C(4A)-C(9A)	119.59(19)
C(5A)-C(4A)-C(3A)	132.62(19)
C(9A)-C(4A)-C(3A)	107.77(16)
C(5B)-C(4B)-C(9B)	119.14(19)
C(5B)-C(4B)-C(3B)	133.44(19)
C(9B)-C(4B)-C(3B)	107.42(17)
C(6A)-C(5A)-C(4A)	118.3(2)
C(6B)-C(5B)-C(4B)	118.6(2)
C(5A)-C(6A)-C(7A)	121.3(2)
C(5B)-C(6B)-C(7B)	121.5(2)
C(8A)-C(7A)-C(6A)	121.6(2)
C(8B)-C(7B)-C(6B)	121.2(2)
C(7A)-C(8A)-C(9A)	116.9(2)
C(7B)-C(8B)-C(9B)	117.7(2)
N(1A)-C(9A)-C(8A)	130.47(18)
N(1A)-C(9A)-C(4A)	107.21(16)
C(8A)-C(9A)-C(4A)	122.31(18)
N(1B)-C(9B)-C(8B)	130.66(19)
N(1B)-C(9B)-C(4B)	107.41(17)
C(8B)-C(9B)-C(4B)	121.93(19)
C(12A)-C(11A)-C(16A)	118.21(17)
C(12A)-C(11A)-P(1A)	117.55(14)
C(16A)-C(11A)-P(1A)	124.17(14)
C(16B)-C(11B)-C(12B)	118.13(19)
C(16B)-C(11B)-P(1B)	124.31(16)
C(12B)-C(11B)-P(1B)	117.54(16)
C(13A)-C(12A)-C(11A)	120.98(18)
C(13B)-C(12B)-C(11B)	120.6(2)
C(12A)-C(13A)-C(14A)	120.19(18)
C(12B)-C(13B)-C(14B)	120.7(2)
C(13A)-C(14A)-C(15A)	119.59(19)
C(15B)-C(14B)-C(13B)	119.3(2)
C(16A)-C(15A)-C(14A)	120.13(18)

C(14B)-C(15B)-C(16B)	120.3(2)
C(15A)-C(16A)-C(11A)	120.90(17)
C(15B)-C(16B)-C(11B)	120.9(2)
C(22A)-C(17A)-C(18A)	118.63(17)
C(22A)-C(17A)-P(1A)	123.83(14)
C(18A)-C(17A)-P(1A)	117.42(14)
C(18B)-C(17B)-C(22B)	118.2(2)
C(18B)-C(17B)-P(1B)	124.52(15)
C(22B)-C(17B)-P(1B)	117.23(16)
C(19A)-C(18A)-C(17A)	120.74(18)
C(19B)-C(18B)-C(17B)	120.95(19)
C(18A)-C(19A)-C(20A)	120.04(19)
C(18B)-C(19B)-C(20B)	119.8(2)
C(21A)-C(20A)-C(19A)	119.82(18)
C(21B)-C(20B)-C(19B)	120.0(2)
C(20A)-C(21A)-C(22A)	120.31(18)
C(20B)-C(21B)-C(22B)	120.26(19)
C(21A)-C(22A)-C(17A)	120.46(18)
C(21B)-C(22B)-C(17B)	120.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k0191. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1A)	26(1)	28(1)	32(1)	-4(1)	-7(1)	-7(1)
P(1B)	30(1)	43(1)	35(1)	-6(1)	-7(1)	-11(1)
N(1A)	28(1)	26(1)	39(1)	-6(1)	-4(1)	-7(1)
N(1B)	33(1)	45(1)	33(1)	-10(1)	-4(1)	-14(1)
C(2A)	30(1)	29(1)	29(1)	-4(1)	-6(1)	-7(1)
C(2B)	33(1)	35(1)	33(1)	-3(1)	-6(1)	-10(1)
C(3A)	35(1)	28(1)	26(1)	-4(1)	-4(1)	-7(1)
C(3B)	35(1)	29(1)	33(1)	-1(1)	-7(1)	-8(1)
C(4A)	33(1)	30(1)	25(1)	-3(1)	-2(1)	-4(1)
C(4B)	39(1)	29(1)	32(1)	3(1)	-10(1)	-12(1)
C(5A)	41(1)	33(1)	48(1)	-5(1)	-2(1)	1(1)
C(5B)	53(1)	40(1)	41(1)	-6(1)	-13(1)	-15(1)
C(6A)	38(1)	45(1)	64(2)	-4(1)	-2(1)	7(1)
C(6B)	57(2)	51(1)	59(2)	-4(1)	-25(1)	-25(1)
C(7A)	25(1)	62(2)	49(1)	-1(1)	-3(1)	-3(1)
C(7B)	40(1)	48(1)	57(2)	6(1)	-18(1)	-19(1)
C(8A)	31(1)	45(1)	35(1)	-4(1)	-2(1)	-10(1)
C(8B)	36(1)	42(1)	43(1)	3(1)	-8(1)	-14(1)
C(9A)	29(1)	34(1)	25(1)	-2(1)	-2(1)	-5(1)
C(9B)	38(1)	35(1)	32(1)	2(1)	-10(1)	-14(1)
C(10A)	46(1)	32(1)	44(1)	-8(1)	-6(1)	-13(1)
C(10B)	43(1)	45(1)	45(1)	-12(1)	-2(1)	-9(1)
C(11A)	26(1)	22(1)	33(1)	-1(1)	-7(1)	-5(1)
C(11B)	28(1)	44(1)	32(1)	-2(1)	-11(1)	-16(1)
C(12A)	24(1)	28(1)	38(1)	-1(1)	-9(1)	-4(1)
C(12B)	50(1)	43(1)	44(1)	-1(1)	-14(1)	-20(1)
C(13A)	24(1)	35(1)	41(1)	-2(1)	-1(1)	-2(1)
C(13B)	60(2)	58(2)	35(1)	7(1)	-13(1)	-30(1)
C(14A)	39(1)	33(1)	32(1)	-2(1)	-4(1)	-4(1)
C(14B)	43(1)	65(2)	31(1)	-5(1)	-7(1)	-28(1)
C(15A)	33(1)	35(1)	37(1)	-2(1)	-14(1)	-6(1)

C(15B)	35(1)	51(1)	37(1)	-9(1)	-6(1)	-13(1)
C(16A)	26(1)	32(1)	35(1)	-1(1)	-8(1)	-8(1)
C(16B)	33(1)	45(1)	33(1)	-1(1)	-10(1)	-10(1)
C(17A)	20(1)	29(1)	33(1)	-2(1)	-9(1)	-4(1)
C(17B)	34(1)	46(1)	25(1)	-7(1)	-1(1)	-17(1)
C(18A)	29(1)	36(1)	34(1)	-5(1)	-8(1)	-9(1)
C(18B)	41(1)	53(1)	36(1)	1(1)	-13(1)	-24(1)
C(19A)	35(1)	42(1)	33(1)	3(1)	-8(1)	-11(1)
C(19B)	57(1)	53(1)	40(1)	3(1)	-20(1)	-21(1)
C(20A)	32(1)	30(1)	48(1)	4(1)	-11(1)	-9(1)
C(20B)	69(2)	46(1)	32(1)	-2(1)	-6(1)	-27(1)
C(21A)	30(1)	30(1)	45(1)	-7(1)	-9(1)	-5(1)
C(21B)	46(1)	56(1)	39(1)	-12(1)	1(1)	-28(1)
C(22A)	25(1)	31(1)	32(1)	-4(1)	-7(1)	-5(1)
C(22B)	33(1)	56(1)	36(1)	-12(1)	-2(1)	-19(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for k0191.

	x	y	z	U(eq)
H(5AA)	2320	10896	1132	53
H(5BA)	968	131	2952	52
H(6AA)	-1	10762	1190	65
H(6BA)	-1439	145	3275	61
H(7AA)	-529	8686	1238	58
H(7BA)	-2948	1145	4373	56
H(8AA)	1252	6666	1236	46
H(8BA)	-2092	2213	5158	49
H(10A)	6529	9165	1027	60
H(10B)	5127	10130	1483	60
H(10C)	5471	10244	534	60
H(10D)	4423	1081	3360	68
H(10E)	3500	1075	2728	68
H(10F)	3843	-219	3364	68
H(12A)	9628	6263	-333	37
H(12B)	3305	1218	6152	52
H(13A)	10271	6350	-1710	43
H(13B)	2343	1630	7463	59
H(14A)	8560	6507	-2455	44
H(14B)	1265	3831	7776	52
H(15A)	6196	6576	-1808	41
H(15B)	1117	5624	6759	48
H(16A)	5548	6494	-431	37
H(16B)	2019	5220	5440	44
H(18A)	6324	4959	2373	39
H(18B)	1355	4589	3783	49
H(19A)	6255	2748	2911	45
H(19B)	1198	6693	3022	57
H(20A)	6839	1048	2077	45
H(20B)	3004	7825	2859	57

H(21A)	7484	1571	707	42
H(21B)	4934	6866	3472	54
H(22A)	7559	3784	162	35
H(22B)	5139	4733	4194	48
H(1A)	4170(20)	5790(30)	1131(14)	51(7)
H(1B)	430(30)	2780(30)	5276(16)	58(8)

Additional Material: [P(C₆H₅)(C₉H₈N)₂] (2)

Table 1. Crystal data and structure refinement for k0457.

Identification code	k0457	
Empirical formula	C ₂₄ H ₂₁ N ₂ P	
Formula weight	368.40	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2(1)/c	
Unit cell dimensions	a = 10.3563(5) Å	α = 90°.
	b = 10.3027(6) Å	β = 104.383(3)°.
	c = 19.0016(8) Å	γ = 90°.
Volume	1963.88(17) Å ³	
Z	4	
Density (calculated)	1.246 Mg/m ³	
Absorption coefficient	0.150 mm ⁻¹	
F(000)	776	
Crystal size	0.20 x 0.18 x 0.18 mm ³	
Theta range for data collection	2.27 to 27.50°.	
Index ranges	-13 ≤ h ≤ 13, -13 ≤ k ≤ 13, -24 ≤ l ≤ 24	
Reflections collected	16135	
Independent reflections	4736 [R(int) = 0.0904]	
Completeness to theta = 27.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.993 and 0.602	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4482 / 0 / 255	
Goodness-of-fit on F ²	1.020	
Final R indices [I > 2σ(I)]	R1 = 0.0546, wR2 = 0.1221	
R indices (all data)	R1 = 0.1017, wR2 = 0.1442	
Extinction coefficient	0.0111(16)	
Largest diff. peak and hole	0.359 and -0.318 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k0457. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
P(1)	7684(1)	5608(1)	1290(1)	29(1)
N(1)	8734(2)	3058(2)	1323(1)	30(1)
N(11)	10464(2)	5613(2)	1954(1)	30(1)
C(2)	7610(2)	3861(2)	1180(1)	29(1)
C(3)	6490(2)	3115(2)	939(1)	29(1)
C(4)	6933(2)	1795(2)	930(1)	28(1)
C(5)	6261(2)	609(2)	752(1)	36(1)
C(6)	7009(3)	-522(2)	810(1)	39(1)
C(7)	8402(3)	-491(2)	1036(1)	39(1)
C(8)	9091(2)	660(2)	1214(1)	34(1)
C(9)	8336(2)	1798(2)	1163(1)	29(1)
C(10)	5078(2)	3576(3)	737(1)	38(1)
C(12)	9431(2)	5890(2)	1346(1)	28(1)
C(13)	9972(2)	6343(2)	799(1)	28(1)
C(14)	11395(2)	6372(2)	1086(1)	30(1)
C(15)	12460(2)	6737(2)	790(1)	36(1)
C(16)	13731(2)	6686(3)	1228(1)	41(1)
C(17)	13982(2)	6272(3)	1951(2)	42(1)
C(18)	12955(2)	5881(2)	2254(1)	37(1)
C(19)	11667(2)	5942(2)	1811(1)	30(1)
C(20)	9243(2)	6707(2)	45(1)	36(1)
C(21)	7637(2)	5804(2)	2247(1)	28(1)
C(22)	7410(2)	4779(2)	2679(1)	32(1)
C(23)	7245(2)	5014(3)	3376(1)	38(1)
C(24)	7301(2)	6273(3)	3641(1)	36(1)
C(25)	7534(2)	7305(2)	3216(1)	35(1)
C(26)	7694(2)	7072(2)	2523(1)	32(1)

Table 3. Bond lengths [Å] and angles [°] for k0457.

P(1)-C(12)	1.809(2)
P(1)-C(2)	1.812(2)
P(1)-C(21)	1.841(2)
N(1)-C(9)	1.373(3)
N(1)-C(2)	1.398(3)
N(11)-C(19)	1.382(3)
N(11)-C(12)	1.395(3)
C(2)-C(3)	1.372(3)
C(3)-C(4)	1.437(3)
C(3)-C(10)	1.494(3)
C(4)-C(5)	1.406(3)
C(4)-C(9)	1.410(3)
C(5)-C(6)	1.388(3)
C(6)-C(7)	1.400(4)
C(7)-C(8)	1.382(3)
C(8)-C(9)	1.398(3)
C(12)-C(13)	1.380(3)
C(13)-C(14)	1.439(3)
C(13)-C(20)	1.491(3)
C(14)-C(19)	1.407(3)
C(14)-C(15)	1.409(3)
C(15)-C(16)	1.373(3)
C(16)-C(17)	1.399(4)
C(17)-C(18)	1.389(3)
C(18)-C(19)	1.390(3)
C(21)-C(22)	1.394(3)
C(21)-C(26)	1.404(3)
C(22)-C(23)	1.397(3)
C(23)-C(24)	1.388(4)
C(24)-C(25)	1.392(3)
C(25)-C(26)	1.388(3)
C(12)-P(1)-C(2)	100.31(10)
C(12)-P(1)-C(21)	101.29(10)

C(2)-P(1)-C(21)	102.22(10)
C(9)-N(1)-C(2)	109.11(18)
C(19)-N(11)-C(12)	109.31(19)
C(3)-C(2)-N(1)	109.1(2)
C(3)-C(2)-P(1)	127.10(17)
N(1)-C(2)-P(1)	123.79(16)
C(2)-C(3)-C(4)	106.75(19)
C(2)-C(3)-C(10)	126.9(2)
C(4)-C(3)-C(10)	126.4(2)
C(5)-C(4)-C(9)	119.2(2)
C(5)-C(4)-C(3)	133.3(2)
C(9)-C(4)-C(3)	107.55(19)
C(6)-C(5)-C(4)	118.5(2)
C(5)-C(6)-C(7)	121.1(2)
C(8)-C(7)-C(6)	121.7(2)
C(7)-C(8)-C(9)	117.1(2)
N(1)-C(9)-C(8)	130.2(2)
N(1)-C(9)-C(4)	107.47(19)
C(8)-C(9)-C(4)	122.3(2)
C(13)-C(12)-N(11)	108.79(18)
C(13)-C(12)-P(1)	126.68(17)
N(11)-C(12)-P(1)	124.46(16)
C(12)-C(13)-C(14)	106.83(19)
C(12)-C(13)-C(20)	127.3(2)
C(14)-C(13)-C(20)	125.9(2)
C(19)-C(14)-C(15)	119.3(2)
C(19)-C(14)-C(13)	107.65(19)
C(15)-C(14)-C(13)	133.1(2)
C(16)-C(15)-C(14)	118.4(2)
C(15)-C(16)-C(17)	121.5(2)
C(18)-C(17)-C(16)	121.4(2)
C(17)-C(18)-C(19)	117.0(2)
N(11)-C(19)-C(18)	130.3(2)
N(11)-C(19)-C(14)	107.34(19)
C(18)-C(19)-C(14)	122.4(2)
C(22)-C(21)-C(26)	118.8(2)

C(22)-C(21)-P(1)	123.31(18)
C(26)-C(21)-P(1)	117.53(17)
C(21)-C(22)-C(23)	120.4(2)
C(24)-C(23)-C(22)	120.1(2)
C(23)-C(24)-C(25)	120.1(2)
C(26)-C(25)-C(24)	119.8(2)
C(25)-C(26)-C(21)	120.8(2)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k0457. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	27(1)	27(1)	32(1)	-1(1)	8(1)	0(1)
N(1)	25(1)	28(1)	38(1)	-3(1)	9(1)	-1(1)
N(11)	28(1)	37(1)	27(1)	4(1)	8(1)	0(1)
C(2)	29(1)	28(1)	29(1)	-1(1)	8(1)	-1(1)
C(3)	29(1)	30(1)	28(1)	-1(1)	9(1)	-1(1)
C(4)	30(1)	29(1)	24(1)	-3(1)	7(1)	-2(1)
C(5)	36(1)	36(1)	34(1)	-5(1)	7(1)	-7(1)
C(6)	48(1)	28(1)	40(1)	-5(1)	7(1)	-6(1)
C(7)	51(1)	31(1)	36(1)	-2(1)	11(1)	8(1)
C(8)	34(1)	35(1)	33(1)	0(1)	9(1)	4(1)
C(9)	32(1)	28(1)	28(1)	0(1)	9(1)	-2(1)
C(10)	28(1)	37(2)	50(2)	-3(1)	10(1)	-2(1)
C(12)	29(1)	24(1)	30(1)	-2(1)	7(1)	-1(1)
C(13)	32(1)	24(1)	30(1)	-2(1)	10(1)	-1(1)
C(14)	33(1)	23(1)	35(1)	-3(1)	13(1)	1(1)
C(15)	40(1)	32(1)	42(1)	-2(1)	21(1)	-1(1)
C(16)	34(1)	39(2)	56(2)	-7(1)	22(1)	-2(1)
C(17)	27(1)	44(2)	54(2)	-10(1)	10(1)	3(1)
C(18)	33(1)	40(2)	37(1)	-4(1)	7(1)	3(1)
C(19)	30(1)	28(1)	34(1)	-4(1)	11(1)	0(1)
C(20)	41(1)	36(1)	30(1)	3(1)	9(1)	3(1)
C(21)	22(1)	28(1)	35(1)	-2(1)	9(1)	0(1)
C(22)	32(1)	28(1)	37(1)	-2(1)	10(1)	-3(1)
C(23)	42(1)	36(2)	39(1)	3(1)	14(1)	-5(1)
C(24)	35(1)	42(2)	35(1)	-3(1)	13(1)	-3(1)
C(25)	35(1)	31(1)	41(1)	-6(1)	12(1)	-2(1)
C(26)	30(1)	32(1)	35(1)	1(1)	11(1)	0(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for k0457.

	x	y	z	U(eq)
H(5A)	5316	581	595	43
H(6A)	6567	-1332	694	47
H(7A)	8887	-1281	1067	47
H(8A)	10037	678	1365	41
H(10A)	5061	4517	659	58
H(10B)	4652	3372	1130	58
H(10C)	4596	3143	290	58
H(15A)	12303	7012	299	43
H(16A)	14458	6937	1036	49
H(17A)	14873	6258	2240	50
H(18A)	13125	5585	2742	44
H(20A)	8282	6715	8	54
H(20B)	9439	6074	-299	54
H(20C)	9528	7572	-69	54
H(22A)	7368	3915	2500	38
H(23A)	7093	4311	3668	46
H(24A)	7180	6431	4113	44
H(25A)	7584	8167	3399	42
H(26A)	7843	7779	2232	38
H(11A)	10420(20)	5440(20)	2369(14)	36(7)
H(1A)	9590(20)	3350(30)	1496(13)	36(7)

Additional Material: P(C₆H₅)₂(C₁₀H₁₀N), (N-Me)-1

Table 1. Crystal data and structure refinement for k0470.

Identification code	k0470	
Empirical formula	C ₂₈ H ₂₄ N P	
Formula weight	405.45	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 13.7780(5) Å	α = 90°
	b = 8.7875(4) Å	β = 105.301(2)°
	c = 18.6350(7) Å	γ = 90°
Volume	2176.24(15) Å ³	
Z	4	
Density (calculated)	1.237 Mg/m ³	
Absorption coefficient	0.141 mm ⁻¹	
F(000)	856	
Crystal size	0.46 x 0.30 x 0.22 mm ³	
Theta range for data collection	2.38 to 27.50°	
Index ranges	-17 ≤ h ≤ 17, -10 ≤ k ≤ 11, -23 ≤ l ≤ 24	
Reflections collected	19191	
Independent reflections	5299 [R(int) = 0.0466]	
Completeness to theta = 27.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.971 and 0.909	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4972 / 0 / 273	
Goodness-of-fit on F ²	1.029	
Final R indices [I > 2σ(I)]	R1 = 0.0520, wR2 = 0.1298	
R indices (all data)	R1 = 0.0866, wR2 = 0.1529	
Extinction coefficient	0.0073(17)	
Largest diff. peak and hole	0.346 and -0.391 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k0470. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
P(1)	2921(1)	7913(1)	1439(1)	42(1)
N(1)	3356(2)	5808(2)	2591(1)	60(1)
C(2)	2598(2)	6694(3)	2131(1)	46(1)
C(3)	1713(2)	6450(2)	2332(1)	47(1)
C(4)	1930(2)	5388(3)	2931(1)	58(1)
C(5)	1350(3)	4750(3)	3369(1)	76(1)
C(6)	1781(4)	3721(4)	3904(2)	105(2)
C(7)	2783(4)	3315(4)	4033(2)	116(2)
C(8)	3399(3)	3941(4)	3628(1)	94(1)
C(9)	2949(3)	4998(3)	3074(1)	68(1)
C(10)	707(2)	7132(3)	2014(1)	55(1)
C(11)	2342(1)	6951(2)	555(1)	36(1)
C(12)	1670(2)	5748(2)	475(1)	43(1)
C(13)	1288(2)	5069(3)	-213(1)	52(1)
C(14)	1581(2)	5576(3)	-825(1)	52(1)
C(15)	2240(2)	6763(3)	-756(1)	50(1)
C(16)	2627(2)	7442(3)	-72(1)	46(1)
C(17)	2084(2)	9533(2)	1434(1)	40(1)
C(18)	1422(2)	10105(2)	794(1)	43(1)
C(19)	853(2)	11402(3)	824(1)	50(1)
C(20)	948(2)	12150(3)	1492(1)	55(1)
C(21)	1600(2)	11600(3)	2130(1)	59(1)
C(22)	2168(2)	10311(3)	2103(1)	52(1)
C(23)	4381(2)	5680(4)	2525(2)	77(1)
C(24)	4469(2)	4749(3)	1866(1)	63(1)
C(25)	3826(2)	3555(3)	1588(1)	57(1)
C(26)	3950(2)	2676(4)	1001(1)	74(1)
C(27)	4730(3)	2995(6)	691(2)	103(2)
C(28)	5361(3)	4187(7)	952(3)	129(2)
C(29)	5230(2)	5064(5)	1536(3)	100(1)

Table 3. Bond lengths [Å] and angles [°] for k0470.

P(1)-C(2)	1.819(2)
P(1)-C(17)	1.831(2)
P(1)-C(11)	1.836(2)
N(1)-C(9)	1.377(3)
N(1)-C(2)	1.400(3)
N(1)-C(23)	1.454(4)
C(2)-C(3)	1.385(3)
C(3)-C(4)	1.425(3)
C(3)-C(10)	1.482(3)
C(4)-C(5)	1.401(4)
C(4)-C(9)	1.401(4)
C(5)-C(6)	1.361(5)
C(6)-C(7)	1.383(6)
C(7)-C(8)	1.390(6)
C(8)-C(9)	1.406(4)
C(11)-C(12)	1.387(3)
C(11)-C(16)	1.395(3)
C(12)-C(13)	1.386(3)
C(13)-C(14)	1.381(3)
C(14)-C(15)	1.367(3)
C(15)-C(16)	1.382(3)
C(17)-C(18)	1.390(3)
C(17)-C(22)	1.400(3)
C(18)-C(19)	1.393(3)
C(19)-C(20)	1.384(3)
C(20)-C(21)	1.374(4)
C(21)-C(22)	1.385(4)
C(23)-C(24)	1.507(4)
C(24)-C(29)	1.376(4)
C(24)-C(25)	1.383(4)
C(25)-C(26)	1.385(4)
C(26)-C(27)	1.378(4)
C(27)-C(28)	1.366(7)
C(28)-C(29)	1.383(7)

C(2)-P(1)-C(17)	100.95(10)
C(2)-P(1)-C(11)	103.60(9)
C(17)-P(1)-C(11)	103.24(9)
C(9)-N(1)-C(2)	108.8(2)
C(9)-N(1)-C(23)	125.9(2)
C(2)-N(1)-C(23)	125.1(2)
C(3)-C(2)-N(1)	108.37(19)
C(3)-C(2)-P(1)	132.94(18)
N(1)-C(2)-P(1)	118.67(17)
C(2)-C(3)-C(4)	107.2(2)
C(2)-C(3)-C(10)	128.8(2)
C(4)-C(3)-C(10)	124.0(2)
C(5)-C(4)-C(9)	119.2(3)
C(5)-C(4)-C(3)	133.2(3)
C(9)-C(4)-C(3)	107.6(2)
C(6)-C(5)-C(4)	119.2(4)
C(5)-C(6)-C(7)	121.3(4)
C(6)-C(7)-C(8)	121.9(3)
C(7)-C(8)-C(9)	116.4(4)
N(1)-C(9)-C(4)	108.1(2)
N(1)-C(9)-C(8)	130.1(3)
C(4)-C(9)-C(8)	121.8(3)
C(12)-C(11)-C(16)	118.28(18)
C(12)-C(11)-P(1)	124.52(14)
C(16)-C(11)-P(1)	117.17(16)
C(13)-C(12)-C(11)	120.48(18)
C(14)-C(13)-C(12)	120.2(2)
C(15)-C(14)-C(13)	120.0(2)
C(14)-C(15)-C(16)	120.09(19)
C(15)-C(16)-C(11)	120.9(2)
C(18)-C(17)-C(22)	118.0(2)
C(18)-C(17)-P(1)	123.73(15)
C(22)-C(17)-P(1)	118.13(17)
C(17)-C(18)-C(19)	120.65(19)
C(20)-C(19)-C(18)	120.3(2)

C(21)-C(20)-C(19)	119.8(2)
C(20)-C(21)-C(22)	120.2(2)
C(21)-C(22)-C(17)	121.1(2)
N(1)-C(23)-C(24)	113.6(2)
C(29)-C(24)-C(25)	118.2(3)
C(29)-C(24)-C(23)	119.3(3)
C(25)-C(24)-C(23)	122.4(2)
C(24)-C(25)-C(26)	121.3(2)
C(27)-C(26)-C(25)	119.3(4)
C(28)-C(27)-C(26)	120.0(4)
C(27)-C(28)-C(29)	120.3(3)
C(24)-C(29)-C(28)	120.8(4)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k0470. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	42(1)	45(1)	38(1)	0(1)	6(1)	-7(1)
N(1)	72(1)	57(1)	36(1)	2(1)	-9(1)	0(1)
C(2)	62(1)	42(1)	30(1)	-4(1)	2(1)	-5(1)
C(3)	77(2)	34(1)	35(1)	-6(1)	21(1)	-9(1)
C(4)	110(2)	34(1)	30(1)	-9(1)	19(1)	-11(1)
C(5)	163(3)	36(1)	42(1)	-13(1)	48(2)	-23(2)
C(6)	234(5)	49(2)	39(2)	-7(1)	46(2)	-29(3)
C(7)	243(6)	60(2)	25(1)	7(1)	0(2)	-23(3)
C(8)	159(3)	64(2)	35(1)	4(1)	-17(2)	-2(2)
C(9)	122(2)	46(1)	24(1)	-1(1)	-1(1)	-9(2)
C(10)	74(2)	42(1)	60(1)	-3(1)	36(1)	-8(1)
C(11)	38(1)	37(1)	34(1)	3(1)	11(1)	4(1)
C(12)	53(1)	44(1)	36(1)	-3(1)	19(1)	-6(1)
C(13)	63(1)	52(1)	45(1)	-13(1)	20(1)	-12(1)
C(14)	65(1)	57(2)	33(1)	-5(1)	11(1)	9(1)
C(15)	70(2)	49(1)	36(1)	10(1)	23(1)	18(1)
C(16)	53(1)	41(1)	49(1)	7(1)	24(1)	3(1)
C(17)	48(1)	36(1)	38(1)	-2(1)	13(1)	-12(1)
C(18)	52(1)	42(1)	37(1)	-3(1)	14(1)	-6(1)
C(19)	60(1)	43(1)	49(1)	4(1)	18(1)	-2(1)
C(20)	81(2)	31(1)	60(1)	-2(1)	34(1)	-6(1)
C(21)	98(2)	34(1)	48(1)	-9(1)	28(1)	-16(1)
C(22)	76(2)	40(1)	38(1)	-5(1)	10(1)	-17(1)
C(23)	60(2)	77(2)	67(2)	11(2)	-31(1)	-5(1)
C(24)	33(1)	82(2)	63(2)	32(1)	-8(1)	4(1)
C(25)	44(1)	90(2)	37(1)	10(1)	8(1)	1(1)
C(26)	60(2)	120(3)	41(1)	6(1)	9(1)	18(2)
C(27)	75(2)	179(4)	67(2)	43(2)	37(2)	62(3)
C(28)	59(2)	186(5)	162(4)	98(4)	65(3)	52(3)
C(29)	32(1)	115(3)	151(3)	59(3)	21(2)	14(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for k0470.

	x	y	z	U(eq)
H(5A)	665	5032	3293	91
H(6A)	1386	3272	4196	126
H(7A)	3057	2588	4409	139
H(8A)	4089	3668	3720	113
H(10A)	659	7488	1507	83
H(10B)	612	7993	2322	83
H(10C)	186	6366	2001	83
H(12A)	1471	5387	895	51
H(13A)	822	4253	-264	63
H(14A)	1324	5100	-1295	62
H(15A)	2433	7122	-1180	60
H(16A)	3094	8255	-27	55
H(18A)	1358	9606	331	52
H(19A)	397	11774	384	60
H(20A)	564	13040	1510	66
H(21A)	1661	12106	2590	70
H(22A)	2622	9949	2546	62
H(23A)	4804	5211	2985	93
H(23B)	4647	6714	2484	93
H(25A)	3289	3334	1803	69
H(26A)	3501	1860	815	89
H(27A)	4830	2387	295	124
H(28A)	5891	4416	732	155
H(29A)	5671	5893	1712	120

Additional Material: [P(C₆H₅)(C₂₃H₂₆N₄)], [(N-CH₂NMe₂)₂-3]

Table 1. Crystal data and structure refinement for k01162a.

Identification code	k01162a	
Empirical formula	C ₂₉ H ₃₁ N ₄ P	
Formula weight	466.55	
Temperature	150(1) K	
Wavelength	0.71070 Å	
Crystal system	Monoclinic	
Space group	P 21/c	
Unit cell dimensions	a = 12.8780(3) Å	α = 90°.
	b = 18.6590(6) Å	β = 116.2791(18)°.
	c = 11.6680(3) Å	γ = 90°.
Volume	2513.94(12) Å ³	
Z	4	
Density (calculated)	1.233 Mg/m ³	
Absorption coefficient	0.134 mm ⁻¹	
F(000)	992	
Crystal size	0.30 x 0.25 x 0.12 mm ³	
Theta range for data collection	2.93 to 25.04°.	
Index ranges	-15 ≤ h ≤ 13, -22 ≤ k ≤ 22, -13 ≤ l ≤ 13	
Reflections collected	17602	
Independent reflections	4431 [R(int) = 0.065]	
Completeness to theta = 25.04°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9841 and 0.9609	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4431 / 0 / 312	
Goodness-of-fit on F ²	1.019	
Final R indices [I > 2σ(I)]	R1 = 0.0473, wR2 = 0.1095	
R indices (all data)	R1 = 0.0725, wR2 = 0.1237	
Extinction coefficient	0.0064(12)	
Largest diff. peak and hole	0.580 and -0.229 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k01162a. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^j tensor.

	x	y	z	$U(\text{eq})$
P(1)	5310(1)	1169(1)	468(1)	28(1)
N(1)	7171(2)	688(1)	24(2)	29(1)
C(2)	5965(2)	770(1)	-470(2)	27(1)
C(3)	5438(2)	472(1)	-1668(2)	27(1)
C(4)	6337(2)	181(1)	-1939(2)	28(1)
C(5)	6336(2)	-178(1)	-2995(2)	32(1)
C(6)	7380(2)	-371(1)	-2964(2)	37(1)
C(7)	8425(2)	-207(1)	-1906(2)	41(1)
C(8)	8456(2)	142(1)	-853(2)	37(1)
C(9)	7398(2)	329(1)	-876(2)	30(1)
C(10)	4174(2)	464(1)	-2550(2)	30(1)
N(11)	2891(2)	1321(1)	-596(2)	28(1)
C(12)	3839(2)	1091(1)	-780(2)	27(1)
C(13)	3450(2)	791(1)	-1969(2)	27(1)
C(14)	2212(2)	836(1)	-2564(2)	28(1)
C(15)	1344(2)	651(1)	-3778(2)	33(1)
C(16)	202(2)	779(1)	-4055(2)	37(1)
C(17)	-100(2)	1081(1)	-3145(2)	38(1)
C(18)	731(2)	1277(1)	-1947(2)	34(1)
C(19)	1890(2)	1161(1)	-1678(2)	29(1)
C(20)	5612(2)	2128(1)	370(2)	28(1)
C(21)	6168(2)	2512(1)	1506(2)	36(1)
C(22)	6448(2)	3230(1)	1489(2)	44(1)
C(23)	6167(2)	3570(1)	342(2)	44(1)
C(24)	5608(2)	3195(1)	-794(2)	40(1)
C(25)	5335(2)	2480(1)	-776(2)	33(1)
C(26)	8021(2)	884(1)	1302(2)	34(1)
N(27)	8922(2)	1354(1)	1301(2)	41(1)
C(28)	8497(2)	1999(1)	554(3)	48(1)
C(29)	9705(2)	1527(2)	2628(2)	55(1)
C(30)	2910(2)	1585(1)	585(2)	31(1)

N(31)	2254(2)	2244(1)	376(2)	31(1)
C(32)	2854(2)	2859(1)	186(2)	38(1)
C(33)	1934(2)	2370(1)	1412(3)	45(1)

Table 3. Bond lengths [Å] and angles [°] for k01162a.

P(1)-C(2)	1.811(2)
P(1)-C(12)	1.814(2)
P(1)-C(20)	1.845(2)
N(1)-C(9)	1.383(3)
N(1)-C(2)	1.404(3)
N(1)-C(26)	1.453(3)
C(2)-C(3)	1.373(3)
C(3)-C(4)	1.434(3)
C(3)-C(10)	1.492(3)
C(4)-C(5)	1.403(3)
C(4)-C(9)	1.408(3)
C(5)-C(6)	1.376(3)
C(6)-C(7)	1.399(3)
C(7)-C(8)	1.376(3)
C(8)-C(9)	1.394(3)
C(10)-C(13)	1.503(3)
N(11)-C(19)	1.379(3)
N(11)-C(12)	1.397(3)
N(11)-C(30)	1.453(3)
C(12)-C(13)	1.368(3)
C(13)-C(14)	1.432(3)
C(14)-C(15)	1.405(3)
C(14)-C(19)	1.410(3)
C(15)-C(16)	1.379(3)
C(16)-C(17)	1.402(3)
C(17)-C(18)	1.381(3)
C(18)-C(19)	1.400(3)
C(20)-C(25)	1.387(3)
C(20)-C(21)	1.393(3)
C(21)-C(22)	1.390(4)
C(22)-C(23)	1.376(4)
C(23)-C(24)	1.384(3)
C(24)-C(25)	1.383(3)
C(26)-N(27)	1.455(3)

N(27)-C(28)	1.444(3)
N(27)-C(29)	1.462(3)
C(30)-N(31)	1.449(3)
N(31)-C(32)	1.455(3)
N(31)-C(33)	1.459(3)
C(2)-P(1)-C(12)	94.72(10)
C(2)-P(1)-C(20)	101.26(10)
C(12)-P(1)-C(20)	101.69(10)
C(9)-N(1)-C(2)	107.97(17)
C(9)-N(1)-C(26)	125.76(18)
C(2)-N(1)-C(26)	126.03(18)
C(3)-C(2)-N(1)	109.41(18)
C(3)-C(2)-P(1)	128.99(16)
N(1)-C(2)-P(1)	121.51(16)
C(2)-C(3)-C(4)	107.10(18)
C(2)-C(3)-C(10)	127.10(19)
C(4)-C(3)-C(10)	125.78(19)
C(5)-C(4)-C(9)	119.3(2)
C(5)-C(4)-C(3)	133.5(2)
C(9)-C(4)-C(3)	107.20(18)
C(6)-C(5)-C(4)	118.8(2)
C(5)-C(6)-C(7)	120.9(2)
C(8)-C(7)-C(6)	121.9(2)
C(7)-C(8)-C(9)	117.3(2)
N(1)-C(9)-C(8)	129.8(2)
N(1)-C(9)-C(4)	108.31(18)
C(8)-C(9)-C(4)	121.9(2)
C(3)-C(10)-C(13)	112.95(18)
C(19)-N(11)-C(12)	108.59(18)
C(19)-N(11)-C(30)	123.87(18)
C(12)-N(11)-C(30)	126.94(17)
C(13)-C(12)-N(11)	109.22(18)
C(13)-C(12)-P(1)	129.08(17)
N(11)-C(12)-P(1)	121.65(16)
C(12)-C(13)-C(14)	107.26(19)

C(12)-C(13)-C(10)	126.97(19)
C(14)-C(13)-C(10)	125.76(19)
C(15)-C(14)-C(19)	119.0(2)
C(15)-C(14)-C(13)	133.8(2)
C(19)-C(14)-C(13)	107.14(19)
C(16)-C(15)-C(14)	118.9(2)
C(15)-C(16)-C(17)	121.1(2)
C(18)-C(17)-C(16)	121.5(2)
C(17)-C(18)-C(19)	117.3(2)
N(11)-C(19)-C(18)	130.1(2)
N(11)-C(19)-C(14)	107.78(18)
C(18)-C(19)-C(14)	122.1(2)
C(25)-C(20)-C(21)	118.6(2)
C(25)-C(20)-P(1)	123.12(17)
C(21)-C(20)-P(1)	118.24(18)
C(22)-C(21)-C(20)	120.6(2)
C(23)-C(22)-C(21)	120.0(2)
C(22)-C(23)-C(24)	120.0(2)
C(25)-C(24)-C(23)	120.0(2)
C(24)-C(25)-C(20)	120.8(2)
N(1)-C(26)-N(27)	112.94(18)
C(28)-N(27)-C(26)	114.45(19)
C(28)-N(27)-C(29)	110.7(2)
C(26)-N(27)-C(29)	108.0(2)
N(31)-C(30)-N(11)	111.40(17)
C(30)-N(31)-C(32)	112.65(17)
C(30)-N(31)-C(33)	110.81(18)
C(32)-N(31)-C(33)	111.29(19)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k01162a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
P(1)	29(1)	28(1)	26(1)	-2(1)	11(1)	2(1)
N(1)	27(1)	28(1)	30(1)	-3(1)	11(1)	1(1)
C(2)	29(1)	23(1)	30(1)	3(1)	14(1)	0(1)
C(3)	32(1)	20(1)	30(1)	1(1)	15(1)	1(1)
C(4)	34(1)	20(1)	32(1)	3(1)	16(1)	1(1)
C(5)	40(1)	25(1)	34(1)	2(1)	18(1)	2(1)
C(6)	48(1)	29(1)	42(1)	-1(1)	27(1)	4(1)
C(7)	39(1)	39(2)	52(2)	-1(1)	26(1)	6(1)
C(8)	32(1)	38(2)	43(1)	-3(1)	18(1)	2(1)
C(9)	34(1)	24(1)	34(1)	0(1)	17(1)	2(1)
C(10)	34(1)	27(1)	28(1)	0(1)	13(1)	3(1)
N(11)	30(1)	28(1)	29(1)	-2(1)	14(1)	0(1)
C(12)	30(1)	23(1)	30(1)	2(1)	15(1)	1(1)
C(13)	31(1)	20(1)	30(1)	1(1)	13(1)	0(1)
C(14)	32(1)	20(1)	31(1)	2(1)	14(1)	-2(1)
C(15)	35(1)	29(1)	33(1)	-1(1)	13(1)	-5(1)
C(16)	33(1)	33(1)	38(1)	-4(1)	9(1)	-9(1)
C(17)	28(1)	35(1)	47(2)	-2(1)	13(1)	-5(1)
C(18)	33(1)	31(1)	43(1)	-1(1)	21(1)	-3(1)
C(19)	30(1)	23(1)	33(1)	0(1)	14(1)	-3(1)
C(20)	27(1)	29(1)	30(1)	-4(1)	13(1)	4(1)
C(21)	38(1)	37(2)	31(1)	-5(1)	13(1)	3(1)
C(22)	47(2)	35(2)	43(2)	-16(1)	12(1)	0(1)
C(23)	48(2)	27(1)	50(2)	-6(1)	16(1)	-2(1)
C(24)	48(2)	31(1)	39(1)	1(1)	16(1)	1(1)
C(25)	34(1)	29(1)	32(1)	-4(1)	11(1)	1(1)
C(26)	31(1)	36(1)	32(1)	1(1)	13(1)	1(1)
N(27)	39(1)	43(1)	36(1)	-3(1)	13(1)	-5(1)
C(28)	45(2)	41(2)	55(2)	2(1)	19(1)	-10(1)
C(29)	44(2)	72(2)	44(2)	-16(2)	15(1)	-13(1)
C(30)	36(1)	30(1)	31(1)	2(1)	18(1)	2(1)

N(31)	34(1)	26(1)	36(1)	-1(1)	19(1)	2(1)
C(32)	48(1)	29(1)	42(1)	1(1)	24(1)	0(1)
C(33)	56(2)	38(2)	57(2)	-2(1)	39(1)	3(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k01162a.

	x	y	z	U(eq)
H(5A)	5629	-285	-3719	39
H(6A)	7391	-618	-3670	44
H(7A)	9133	-341	-1914	49
H(8A)	9169	252	-138	45
H(10A)	3923	-38	-2793	36
H(10B)	4038	729	-3339	36
H(15A)	1540	440	-4398	39
H(16A)	-389	660	-4878	45
H(17A)	-895	1151	-3356	46
H(18A)	524	1483	-1332	41
H(21A)	6359	2280	2299	44
H(22A)	6832	3487	2268	53
H(23A)	6356	4061	329	53
H(24A)	5412	3430	-1585	49
H(25A)	4954	2226	-1559	40
H(26A)	8385	442	1784	40
H(26B)	7623	1126	1751	40
H(28A)	7958	1872	-325	72
H(28B)	9149	2269	553	72
H(28C)	8096	2294	928	72
H(29A)	10333	1834	2652	82
H(29B)	10031	1084	3102	82
H(29C)	9276	1781	3019	82
H(30A)	2580	1217	940	37
H(30B)	3722	1672	1217	37
H(32A)	3036	2765	-531	57
H(32B)	3573	2943	-963	57
H(32C)	2357	3283	-2	57
H(33A)	1527	1949	1514	67
H(33B)	1426	2789	1211	67

H(33C)

2634

2456

2209

67

Additional Material: P(C₆H₅)(C₃₁H₁₄F₁₀N₂), (N-F₅Bz)₂-3

Table 1. Crystal data and structure refinement for k0462.

Identification code	k0462	
Empirical formula	C ₃₈ H ₂₀ Cl ₃ F ₁₀ N ₂ P	
Formula weight	831.88	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 16.5993(5) Å	α = 90°.
	b = 12.0034(3) Å	β = 98.8110(17)°.
	c = 17.1393(4) Å	γ = 90°.
Volume	3374.67(15) Å ³	
Z	4	
Density (calculated)	1.637 Mg/m ³	
Absorption coefficient	0.409 mm ⁻¹	
F(000)	1672	
Crystal size	0.32 x 0.30 x 0.22 mm ³	
Theta range for data collection	1.59 to 27.53°.	
Index ranges	-21 ≤ h ≤ 21, -15 ≤ k ≤ 15, -22 ≤ l ≤ 22	
Reflections collected	32929	
Independent reflections	8134 [R(int) = 0.0528]	
Completeness to theta = 27.53°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.964 and 0.852	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	7756 / 0 / 488	
Goodness-of-fit on F ²	1.027	
Final R indices [I > 2σ(I)]	R1 = 0.0438, wR2 = 0.1071	
R indices (all data)	R1 = 0.0721, wR2 = 0.1221	
Extinction coefficient	0.0013(4)	
Largest diff. peak and hole	0.367 and -0.494 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for k0462. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
P(1)	5500(1)	4858(1)	1201(1)	23(1)
N(1)	3831(1)	4998(1)	1271(1)	24(1)
N(11)	6823(1)	5911(1)	677(1)	24(1)
C(2)	4520(1)	5537(2)	1075(1)	24(1)
C(3)	4291(1)	6543(2)	720(1)	23(1)
C(4)	3423(1)	6630(2)	683(1)	24(1)
C(5)	2846(1)	7427(2)	364(1)	29(1)
C(6)	2034(1)	7231(2)	398(1)	33(1)
C(7)	1783(1)	6266(2)	752(1)	34(1)
C(8)	2336(1)	5468(2)	1077(1)	31(1)
C(9)	3156(1)	5658(2)	1029(1)	26(1)
C(10)	4825(1)	7360(2)	387(1)	24(1)
C(12)	6006(1)	5996(2)	776(1)	23(1)
C(13)	5693(1)	6981(2)	459(1)	23(1)
C(14)	6347(1)	7554(2)	162(1)	24(1)
C(15)	6403(1)	8560(2)	-243(1)	28(1)
C(16)	7133(1)	8831(2)	-490(1)	32(1)
C(17)	7811(1)	8123(2)	-342(1)	32(1)
C(18)	7778(1)	7133(2)	62(1)	28(1)
C(19)	7040(1)	6858(2)	307(1)	24(1)
C(20)	5876(1)	5038(2)	2263(1)	23(1)
C(21)	5680(1)	5937(2)	2708(1)	31(1)
C(22)	5994(2)	6015(2)	3504(1)	34(1)
C(23)	6512(1)	5199(2)	3860(1)	31(1)
C(24)	6716(1)	4296(2)	3424(1)	30(1)
C(25)	6393(1)	4215(2)	2633(1)	26(1)
C(26)	3799(1)	3848(2)	1527(1)	26(1)
C(27)	4149(1)	3636(2)	2386(1)	24(1)
C(28)	3992(1)	4305(2)	3004(1)	29(1)
C(29)	4321(1)	4088(2)	3778(1)	33(1)
C(30)	4806(1)	3169(2)	3958(1)	33(1)

C(31)	4965(1)	2476(2)	3362(1)	33(1)
C(32)	4640(1)	2717(2)	2594(1)	28(1)
C(33)	7376(1)	5029(2)	975(1)	25(1)
C(34)	7867(1)	5212(2)	1786(1)	24(1)
C(35)	7818(1)	6098(2)	2293(1)	26(1)
C(36)	8276(1)	6138(2)	3037(1)	31(1)
C(37)	8808(1)	5293(2)	3292(1)	35(1)
C(38)	8872(1)	4396(2)	2804(1)	35(1)
C(39)	8410(1)	4374(2)	2071(1)	30(1)
C(40)	11149(2)	3274(2)	2476(2)	47(1)
F(28)	3511(1)	5200(1)	2861(1)	45(1)
F(29)	4162(1)	4762(1)	4360(1)	51(1)
F(30)	5113(1)	2942(1)	4709(1)	48(1)
F(31)	5438(1)	1576(1)	3529(1)	55(1)
F(32)	4826(1)	2033(1)	2022(1)	43(1)
F(35)	7312(1)	6964(1)	2087(1)	34(1)
F(36)	8201(1)	7006(1)	3516(1)	44(1)
F(37)	9262(1)	5338(1)	4009(1)	51(1)
F(38)	9381(1)	3554(1)	3045(1)	50(1)
F(39)	8480(1)	3489(1)	1604(1)	40(1)
Cl(41)	12143(1)	2783(1)	2489(1)	54(1)
Cl(42)	10613(1)	3224(1)	1513(1)	63(1)
Cl(43)	11147(1)	4633(1)	2849(1)	76(1)

Table 3. Bond lengths [Å] and angles [°] for k0462.

P(1)-C(2)	1.802(2)
P(1)-C(12)	1.813(2)
P(1)-C(20)	1.844(2)
N(1)-C(9)	1.383(3)
N(1)-C(2)	1.399(3)
N(1)-C(26)	1.452(3)
N(11)-C(19)	1.378(3)
N(11)-C(12)	1.396(3)
N(11)-C(33)	1.442(3)
C(2)-C(3)	1.378(3)
C(3)-C(4)	1.436(3)
C(3)-C(10)	1.494(3)
C(4)-C(5)	1.404(3)
C(4)-C(9)	1.410(3)
C(5)-C(6)	1.378(3)
C(6)-C(7)	1.400(3)
C(7)-C(8)	1.384(3)
C(8)-C(9)	1.395(3)
C(10)-C(13)	1.497(3)
C(12)-C(13)	1.370(3)
C(13)-C(14)	1.442(3)
C(14)-C(15)	1.403(3)
C(14)-C(19)	1.412(3)
C(15)-C(16)	1.382(3)
C(16)-C(17)	1.402(3)
C(17)-C(18)	1.381(3)
C(18)-C(19)	1.394(3)
C(20)-C(21)	1.389(3)
C(20)-C(25)	1.396(3)
C(21)-C(22)	1.386(3)
C(22)-C(23)	1.382(3)
C(23)-C(24)	1.387(3)
C(24)-C(25)	1.382(3)
C(26)-C(27)	1.519(3)